

frac. valid SMILES

0.75  
0.50  
0.25

frac. unique SMILES

1.0  
0.5

frac. SMILES in train

0.05  
0.00  
-0.05

frac. SMILES in PubChem

1.05  
1.00  
0.95

KLD

0.8  
0.6

Frechet distance

50  
25

frac. SMILES with azo

1.0  
0.5

SA score

5  
4  
3

0.0  
0.5  
1.0  
1.5  
2.0

temperature

